

Terephthalic acid, pentyl 2,2,2-trifluoroethyl ester

Inchi:	InChI=1S/C15H17F3O4/c1-2-3-4-9-21-13(19)11-5-7-12(8-6-11)14(20)22-10-15(16,17)18
InchiKey:	UQHZIHSHGMMHNKB-UHFFFAOYSA-N
Formula:	C15H17F3O4
SMILES:	CCCCCOC(=O)c1ccc(C(=O)OCC(F)(F)F)cc1
Mol. weight [g/mol]:	318.29

Physical Properties

Property code	Value	Unit	Source
gf	-871.23	kJ/mol	Joback Method
hf	-1214.55	kJ/mol	Joback Method
hfus	35.66	kJ/mol	Joback Method
hvap	66.49	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	3.753		Crippen Method
mcvol	218.640	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
rinpol	2024.00		NIST Webbook
rinpol	2024.00		NIST Webbook
tb	721.42	K	Joback Method
tc	912.88	K	Joback Method
tf	446.26	K	Joback Method
vc	0.859	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.55	J/molxK	721.42	Joback Method
cpg	632.98	J/molxK	753.33	Joback Method
cpg	645.53	J/molxK	785.24	Joback Method
cpg	657.25	J/molxK	817.15	Joback Method
cpg	668.14	J/molxK	849.06	Joback Method
cpg	678.24	J/molxK	880.97	Joback Method
cpg	687.57	J/molxK	912.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383040&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/115-318-1/Terephthalic-acid-pentyl-2-2-2-trifluoroethyl-ester.pdf>

Generated by Cheméo on 2024-04-29 15:34:41.273651006 +0000 UTC m=+16694130.194228322.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.